

Size quantization of charge carriers in lead salt cylindrical quantum wires

S.V. Goupalov

Department of Physics, Jackson State University, Jackson, MS 39217 USA

and A.F. Ioffe Physico-Technical Institute,

26 Polytechnicheskaya, 194021 St. Petersburg, Russia

Abstract

A formalism for determining energy eigenstates of cylindrical lead salt quantum wires in the multiple-band envelope-function approximation is developed. Electron energy dispersion for quantum wire subbands within the conduction and valence bands is found.

PACS numbers: 73.21.Hb, 73.22.Dj, 78.67.Lt

The effect of quantum confinement on electron and hole states in spherical quantum dots and cylindrical quantum wires of III-V and II-VI semiconductor compounds having a complex valence-band structure was described within the multiband envelope-function approximation more than 20 years ago [1]. Description of electronic structure of spherical IV-VI semiconductor quantum dots using similar approximation followed soon [2]. Recently nanostructures based on IV-VI semiconductor compounds such as lead salts received much attention due to their potential for applications in solar cells and as infra-red detectors. Quasi-zero-dimensional nanostructures of lead salts have become the subject of wave-function engineering [3, 4], and there appeared an interest in quasi-one-dimensional nanostructures of IV-VI semiconductors [5]. However, one is forced to accept the fact that a recent attempt [5] to describe electronic structure of a cylindrical lead salt quantum wire within a multiband envelope-function formalism is not quite correct. This Brief Report seeks to compensate for this deficiency.

The conduction and valence band extrema in lead salt semiconductors (PbSe, PbS) occur at the L -points of the Brillouin zone. Electron spectrum near the L -point taking into account only the two closely lying conduction and valence bands and neglecting band anisotropy can be described by the spherical Dimmock model [2, 6–8]. In this model the electron wave function is written as

$$\Psi = \hat{u} |L_6^-\rangle + \hat{v} |L_6^+\rangle, \quad (1)$$

where $|L_6^-\rangle$ and $|L_6^+\rangle$ describe the Bloch functions while $\hat{u}(\mathbf{r})$ and $\hat{v}(\mathbf{r})$ are the spinors slowly varying with coordinates and satisfying the equations [9]

$$\begin{bmatrix} \left(\frac{E_g}{2} - \alpha_c \Delta\right) & -iP(\boldsymbol{\sigma} \nabla) \\ -iP(\boldsymbol{\sigma} \nabla) & -\left(\frac{E_g}{2} - \alpha_v \Delta\right) \end{bmatrix} \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix} = E \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix}. \quad (2)$$

Here σ_β ($\beta = x, y, z$) are the Pauli matrices, α_c , α_v , E_g , and P are parameters of the model and E is the electron energy.

We will first construct linearly independent solutions of Eqs. (2) having cylindrical symmetry and describing electronic states in a bulk semiconductor. These solutions can be characterized by the energy, E , momentum, k_z along the quantum wire axis, and projection, M of the total angular momentum on the wire axis. Then we will impose the boundary condition of the four-component envelope wave function vanishing on the cylindrical surface

of the quantum wire. In the cylindrical coordinates (ρ, φ, z) this boundary condition is to be imposed at $\rho = R$, where R is the radius of the cylindrical quantum wire.

The high symmetry of the problem allows us to separate variables and pin down a set of good quantum numbers (E , k_z , and M). After this Eqs. (2) can be considered as a system of four coupled ordinary linear differential equations of second order with respect to the variable ρ . As we are only interested in solutions of Eqs. (2) finite at $\rho = 0$, there are at most four such linearly independent solutions of Eqs. (2).

Let us look for a solution of Eqs. (2) in the form

$$\hat{u}_M(\rho, \varphi, z) = e^{ik_z z} \begin{bmatrix} A e^{i(M-1/2)\varphi} J_{M-1/2}(k\rho) \\ B e^{i(M+1/2)\varphi} J_{M+1/2}(k\rho) \end{bmatrix}, \quad (3)$$

$$\hat{v}_M(\rho, \varphi, z) = e^{ik_z z} \begin{bmatrix} C e^{i(M-1/2)\varphi} J_{M-1/2}(k\rho) \\ D e^{i(M+1/2)\varphi} J_{M+1/2}(k\rho) \end{bmatrix}, \quad (4)$$

where $J_n(x)$ is the Bessel function of order n , k is the wave number of transverse motion, and A , B , C , and D are the coefficients to be determined. Substitution of Eqs. (3), (4) into Eqs. (2) leads to a system of the following algebraic equations:

$$P k_z A - i P k B - (\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2) C = 0, \quad (5)$$

$$i P k A - P k_z B - (\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2) D = 0, \quad (6)$$

$$(\alpha_c k^2 + \alpha_c k_z^2 - E + E_g/2) A + P k_z C - i P k D = 0, \quad (7)$$

$$(\alpha_c k^2 + \alpha_c k_z^2 - E + E_g/2) B + i P k C - P k_z D = 0. \quad (8)$$

The condition that this system of algebraic equations has a non-trivial solution yields

$$k^2 + k_z^2 = \Xi + \Lambda, \quad (9)$$

where

$$\Lambda = \frac{E(\alpha_v - \alpha_c) - P^2 - E_g(\alpha_v + \alpha_c)/2}{2\alpha_c\alpha_v},$$

$$\Xi = \frac{\sqrt{[E(\alpha_v - \alpha_c) - E_g(\alpha_v + \alpha_c)/2 - P^2]^2 + \alpha_c\alpha_v(4E^2 - E_g^2)}}{2\alpha_c\alpha_v}.$$

Equations (5), (6) allow one to express the coefficients C and D in terms of A and B :

$$C = \frac{P(k_z A - i k B)}{\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2},$$

$$D = \frac{P(i k A - k_z B)}{\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2}.$$

We see that a natural choice of the two linearly independent solutions will be to set either A or B equal to zero. The resulting solutions (which turn out to be orthogonal) take the form

$$\hat{u}_M^{(1)}(\rho, \varphi, z) = A e^{i k_z z} \begin{bmatrix} e^{i(M-1/2)\varphi} J_{M-1/2}(k\rho) \\ 0 \end{bmatrix}, \quad (10)$$

$$\hat{v}_M^{(1)}(\rho, \varphi, z) = \frac{i P A e^{i k_z z}}{\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2} \begin{bmatrix} -i k_z e^{i(M-1/2)\varphi} J_{M-1/2}(k\rho) \\ k e^{i(M+1/2)\varphi} J_{M+1/2}(k\rho) \end{bmatrix}, \quad (11)$$

$$\hat{u}_M^{(2)}(\rho, \varphi, z) = B e^{i k_z z} \begin{bmatrix} 0 \\ e^{i(M+1/2)\varphi} J_{M+1/2}(k\rho) \end{bmatrix}, \quad (12)$$

$$\hat{v}_M^{(2)}(\rho, \varphi, z) = \frac{i P B e^{i k_z z}}{\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2} \begin{bmatrix} -k e^{i(M-1/2)\varphi} J_{M-1/2}(k\rho) \\ i k_z e^{i(M+1/2)\varphi} J_{M+1/2}(k\rho) \end{bmatrix}. \quad (13)$$

The two remaining solutions of Eqs. (2) can be sought in the form

$$\hat{u}_M(\rho, \varphi, z) = e^{i k_z z} \begin{bmatrix} C e^{i(M-1/2)\varphi} I_{M-1/2}(\kappa\rho) \\ D e^{i(M+1/2)\varphi} I_{M+1/2}(\kappa\rho) \end{bmatrix}, \quad (14)$$

$$\hat{v}_M(\rho, \varphi, z) = e^{i k_z z} \begin{bmatrix} F e^{i(M-1/2)\varphi} I_{M-1/2}(\kappa\rho) \\ G e^{i(M+1/2)\varphi} I_{M+1/2}(\kappa\rho) \end{bmatrix}, \quad (15)$$

where $I_n(x)$ is the modified Bessel function of order n while C , D , F , and G represent a new set of the coefficients to be determined. Substitution of Eqs. (14), (15) into Eqs. (2) yields

$$P k_z C - i P \kappa D + (\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2) F = 0, \quad (16)$$

$$-i P \kappa C - P k_z D + (\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2) G = 0, \quad (17)$$

$$(\alpha_c k_z^2 - \alpha_c \kappa^2 - E + E_g/2) C + P k_z F - i P \kappa G = 0, \quad (18)$$

$$(\alpha_c k_z^2 - \alpha_c \kappa^2 - E + E_g/2) D - i P \kappa F - P k_z G = 0. \quad (19)$$

The condition that this system of algebraic equations has a non-trivial solution yields

$$\kappa^2 - k_z^2 = \Xi - \Lambda. \quad (20)$$

Equations (16), (17) allow one to express the coefficients F and G in terms of C and D :

$$F = \frac{P(-k_z C + i \kappa D)}{\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2},$$

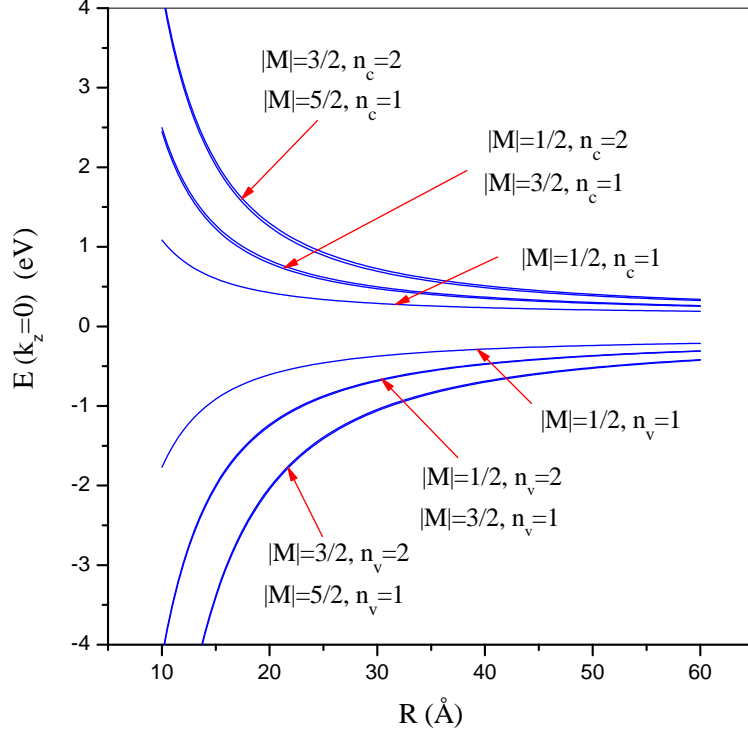


FIG. 1: (Color online) Energy of electron states in PbSe cylindrical quantum wire at $k_z = 0$ as a function of the wire radius.

$$G = \frac{P(i\kappa C + k_z D)}{\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2}.$$

By setting zero either C or D we arrive to the following solutions of Eqs. (2)

$$\hat{u}_M^{(3)}(\rho, \varphi, z) = C e^{ik_z z} \begin{bmatrix} e^{i(M-1/2)\varphi} I_{M-1/2}(\kappa\rho) \\ 0 \end{bmatrix}, \quad (21)$$

$$\hat{v}_M^{(3)}(\rho, \varphi, z) = \frac{iPC e^{ik_z z}}{\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2} \begin{bmatrix} i k_z e^{i(M-1/2)\varphi} I_{M-1/2}(\kappa\rho) \\ \kappa e^{i(M+1/2)\varphi} I_{M+1/2}(\kappa\rho) \end{bmatrix}, \quad (22)$$

$$\hat{u}_M^{(4)}(\rho, \varphi, z) = D e^{ik_z z} \begin{bmatrix} 0 \\ e^{i(M+1/2)\varphi} I_{M+1/2}(\kappa\rho) \end{bmatrix}, \quad (23)$$

$$\hat{v}_M^{(4)}(\rho, \varphi, z) = \frac{iPD e^{ik_z z}}{\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2} \begin{bmatrix} \kappa e^{i(M-1/2)\varphi} I_{M-1/2}(\kappa\rho) \\ -i k_z e^{i(M+1/2)\varphi} I_{M+1/2}(\kappa\rho) \end{bmatrix}. \quad (24)$$

The four solutions we constructed are not mutually orthogonal but they are linearly independent. If one requires that their linear combination (with the coefficients A , B , C , and D) vanishes at $\rho = R$ then one will obtain a system of four homogeneous algebraic equations on these coefficients. The condition that this system has a non-trivial solution will

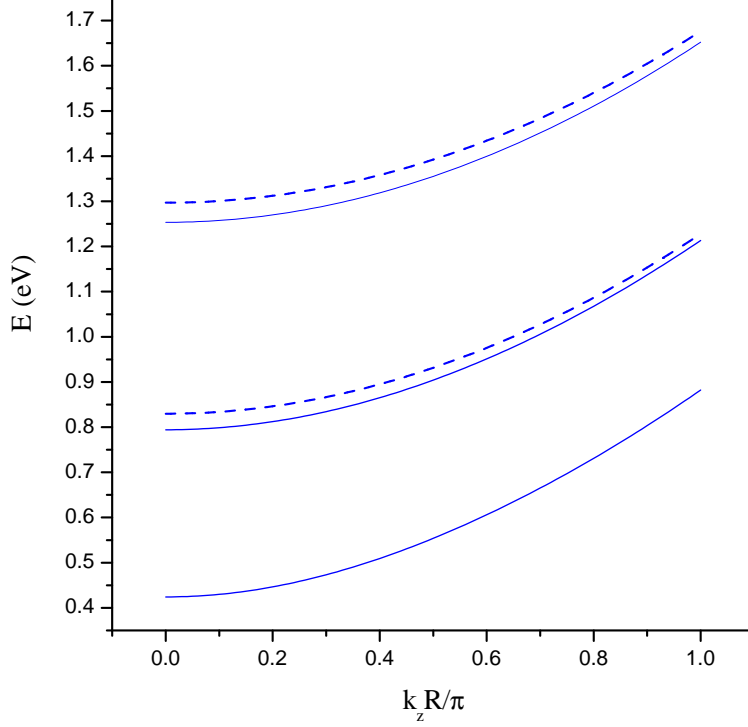


FIG. 2: (Color online) Energy dispersion of electron subbands within the conduction band of a PbSe cylindrical quantum wire of radius $R = 20$ Å. By dashed lines are shown subbands with the quantum number $n_c = 2$.

lead to the dispersion equation determining the allowed energy values of electrons confined in a cylindrical quantum wire. The positive (negative) values of energy describe the states in the conduction (valence) band. The dispersion equation takes the form

$$\begin{aligned}
& \alpha_v^2 k_z^2 (k^2 + \kappa^2)^2 J_{M-1/2}(kR) J_{M+1/2}(kR) I_{M-1/2}(\kappa R) I_{M+1/2}(\kappa R) \\
& + \left[k (\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2) J_{M-1/2}(kR) I_{M+1/2}(\kappa R) \right. \\
& \left. + \kappa (\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2) J_{M+1/2}(kR) I_{M-1/2}(\kappa R) \right] \\
& \times \left[k (\alpha_v \kappa^2 - \alpha_v k_z^2 - E - E_g/2) J_{M+1/2}(kR) I_{M-1/2}(\kappa R) \right. \\
& \left. - \kappa (\alpha_v k^2 + \alpha_v k_z^2 + E + E_g/2) J_{M-1/2}(kR) I_{M+1/2}(\kappa R) \right] = 0.
\end{aligned} \tag{25}$$

In order to better understand the structure of this equation let us first consider the case of $k_z = 0$. In this limit each of the spinors $\hat{u}_M^{(i)}$, $\hat{v}_M^{(i)}$ ($i = 1, 2, 3, 4$) has only one non-zero component. Therefore, for every i the corresponding bispinor solution has two non-zero

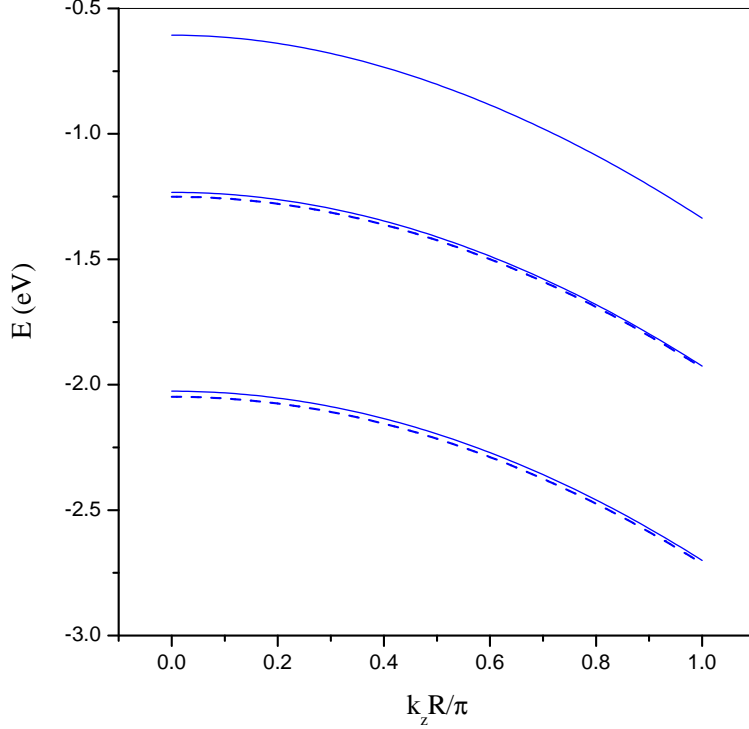


FIG. 3: (Color online) Energy dispersion of electron subbands within the valence band of a PbSe cylindrical quantum wire of radius $R = 20$ Å. By dashed lines are shown subbands with the quantum number $n_v = 2$.

components. Taking into account the parity of the Bloch functions $|L_6^\mp\rangle$, the solutions with $i = 1$ and $i = 3$ have in the limit $k_z = 0$ the parity $(-1)^{M+1/2}$, while the solutions with $i = 2$ and $i = 4$ have the parity $(-1)^{M-1/2}$. The first term of Eq. (25) vanishes in the limit $k_z = 0$, and Eq. (25) reduces to a product of the two square brackets. The first (second) square bracket is responsible for the solutions with the parity $(-1)^{M\mp 1/2}$. This situation is analogous to the case of spherical quantum dots [2, 8].

When $k_z \neq 0$ then each bispinor solution we constructed has three non-zero components. In this case the first term in Eq. (25) does not vanish and factorization of the dispersion equation becomes impossible. This observation is in contradiction with the conclusions of Ref. [5].

Because of the Kramers degeneracy Eq. (25) must be invariant under the change of M to $-M$. This invariance is guaranteed by the properties of the Bessel functions: $J_{-n}(x) = (-1)^n J_n(x)$; $I_{-n}(x) = I_n(x)$.

Let us illustrate our results by numerical calculations. In Fig. 1 are shown energies of electron states in a PbSe cylindrical quantum wire at $k_z = 0$ as a function of the wire radius. Only dependences for the five lowest subbands in the conduction band and five uppermost subbands in the valence band are shown. All the material parameters are taken from Ref. [2]. The electron states in the conduction (valence) band are characterized by the projection, M of the total angular momentum onto the wire axis and by the main quantum number n_c (n_v).

In Fig. 2 (Fig. 3) is shown energy dispersion of electron subbands within the conduction (valence) band of a PbSe cylindrical quantum wire of radius $R = 20$ Å. The solid lines refer to the subbands with the main quantum number $n_{c(v)} = 1$ while the dashed lines refer to the subbands with the main quantum number $n_{c(v)} = 2$. The dependences shown in Figs. 2, 3 are nearly parabolic.

To summarize, we have studied electronic structure of cylindrical lead salt quantum wires within the multi-band envelope-function formalism. We have found the energy dispersion for subbands within the conduction and valence bands of the quantum wire. When applied to real structures, the parameters of the model may be modified for each particular L -valley to reflect its orientation with respect to the quantum wire growth direction and taking into account the valley anisotropy.

The author wishes to thank A.N. Poddubny for useful discussions. This work was supported in part by the NSF under grant No. HRD-0833178 and in part by the Russian Foundation for Basic Research.

-
- [1] P.C. Sercel and K.J. Vahala, Phys. Rev B **42**, 3690 (1990).
 - [2] I. Kang and F.W. Wise, J. Opt. Soc. Am. B **14**, 1632 (1997).
 - [3] A.C. Bartnik, F.W. Wise, A. Kigel, and E. Lifshitz, Phys. Rev. B **75**, 245424 (2007).
 - [4] G.A. Grinbom, M. Saraf, C. Saguy, A.C. Bartnik, F. Wise, and E. Lifshitz, Phys. Rev. B **81**, 245301 (2010).
 - [5] V.I. Rupasov, Phys. Rev. B **80**, 115306 (2009).
 - [6] J.O. Dimmock, in *The Physics of Semimetals and Narrow-Gap Semiconductors*, D.L. Carter

and R.T. Bates, eds. (Pergamon, Oxford, 1971).

[7] L.A. Falkovsky, Physics – Uspekhi **51**, 887 (2008) [Uspekhi Fiz. Nauk **178**, 923 (2008)].

[8] S.V. Goupalov, Phys. Rev. B **79**, 233305 (2009).

[9] We use the system of units where $\hbar = m_0 = e = 1$ (m_0 and e are the mass and the charge of a free electron).